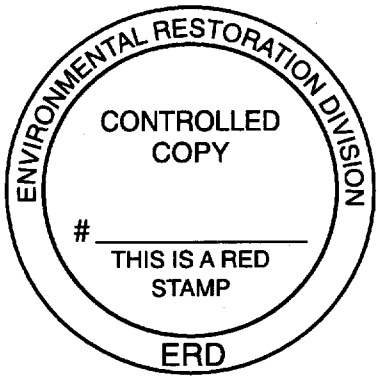
LLNL Environmental Restoration Division (ERD)
Standard Operating Procedure (SOP)

ERD SOP 5.3: Data Management Electronic Analytical Result Receipt and Processing for Sample and Analysis Data—Revision: 1



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1.0 PURPOSE

The purpose of this procedure is to establish the means for receiving and storing electronic analytical results as received from analytical laboratories. This procedure is to ensure complete and consistent handling of all electronic analytical records within the Environmental Restoration Division (ERD) Data Management Team (DMT).

2.0 APPLICABILITY

This procedure applies to DMT personnel performing quality affecting activities in the receipt and storage of electronic analytical results

3.0 REFERENCES

Not applicable.

4.0 DEFINITIONS

See SOP Glossary.

5.0 RESPONSIBILITIES

5.1 Division Leader

The Division Leader has the responsibility for providing the necessary equipment and resources to accomplish the task(s) described by this procedure.

5.2 Data Qualifier Flag Verification Officer

The person responsible for verifying that the electronically recorded data qualifier flags agree with flags assigned by the QC Chemists.

5.3 Validation Recording Officer

The person who is responsible for updating the validation field in the sample table when validation of that sample has been confirmed.

6.0 PROCEDURE

6.1 Establish a Log File

Establish a log file to record details pertinent to the upload being done. Add to this log often throughout the process as each step is completed or as any relevant intermediate steps are completed.

6.2 Copy the Files to a Personal Directory

6.2.1 ERD incorporates data files for ERD and for the Operations and Regulatory Affairs Division (ORAD)Environmental Operations Group (EOG) of EPD from each of the laboratories sending data electronically that are to be stored in the EPDData database. The files are transmitted to the EPD LLNL Wonderland domain. Each laboratory has its own directory. In each transmittal there are 4 files each for ERD and ORAD: Sample, Analysis, QAQC, and Batch Number Reference. The files are in the analytical laboratory's directory, and are named as follows:

ERD	zzerdyymmddsample.xfer	(ERD sample file)
ERD	zzerdyymmddanalysis.xfer	(ERD analysis file)
ERD	zzerdyymmddqaqc1.xfer	(ERD qaqc file)
ERD	zzerdyymmddqaqc2.xfer	(ERD batch number file)
ORAD	zzoradmmddsample.xfer	(ORAD sample file)
ORAD	zzoradmmddanalysis.xfer	(ORAD analysis file)
ORAD	zzoradmmddqaqc1.xfer	(ORAD qaqc file)
ORAD	zzoradmmddqaqc2.xfer	(ORAD batch number file)

Where: ZZ=two letter code for the laboratory

YY=year

MM=month

DD=day.

Note: The date should be the same for all eight files.

6.2.2 Copy files into your account, using one of the following examples.

- Use this example if you are concatenating two files:

  % cat zzerdyymmddsamp.xfer zzoradyymmddsamp.xfer | dos2unix > /home/[your HOME dir]/sample.xfer

  % cat zzerdyymmddanal.xfer zzoradyymmddanal.xfer | dos2unix > /home/[your HOME dir]/analysis.xfer

  % cat zzerdyymmddqaqc1.xfer zzoradyymmddqaqc1.xfer | dos2unix > /home/[your HOME dir]/qaqc1.xfer

  % cat zzerdyymmddqaqc2.xfer zzoradyymmddqaqc2.xfer | dos2unix > /home/[your HOME dir]/qaqc2.xfer

- Use this example if you are only copying single files:

  % cp zzerdyymmddsamp.xfer | dos2unix > /home/[your HOME dir] /sample.xfer

  % cp zzerdyymmddanal.xfer | dos2unix > /home/[your HOME dir] /analysis.xfer

  % cp zzerdyymmddqaqc1.xfer | dos2unix > /home/[your HOME dir] /qaqc1.xfer

  % cp zzerdyymmddqaqc2.xfer | dos2unix > /home/[your HOME dir] /qaqc2.xfer

6.2.3 Convert files in the lab's directory to have the extension of .DMT when copy is complete. Example:

% mv zzerdyymmddsamp.xfer zzerdyymmddsamp.DMT

6.2.4 Count and record the number of rows in each file (you will see the count in the lower left corner of screen):

Note: The numbers represent a line count. Example:

%wc -l sample.xfer

6.2.5 Run CHECK CHARACTER program on the sample.xfer, analysis.xfer, qaqc1.xfer, and qaqc2.xfer files using the following UNIX commands:

% chkcharsample.xfer > chkcharsamp.log

% chkcharanalysis.xfer > chkcharanal.log

% chkcharqaqc1.xfer > chkcharqaqc1.log

% chkcharqaqc2.xfer > chkcharqaqc2.log

- Visually scan output files in your home directory for a report of illegal characters. Make adjustments if there are any illegal characters (*, %, ?, #, ^Z, _, /) that might prevent the upload into INGRES.

6.2.6 Determine whether each file has the correct number of delimiters. Run the Count Delimiters program on all files. Use the following UNIX command: % dmg cntdlm [file name]

The 4 files should contain the following number of delimiters:

sample.xfer 8

analysis.xfer 20

qaqc1.xfer 33

qaqc2.xfer 1

6.2.7 Identify TICs, as necessary, by the analyte type field in the analysis file, change from TRG to TIC.

6.3 Upload Data

6.3.1 Ensure your work tables have zero rows:

wsample

wanalysis

wqcanal

wqckey

wtic_analysis

wsur_analysis

wanal_comments

6.3.2 Upload sample and analysis data to your working tables using the monitor application. From the monitor menu select:

C1 Convert Work Tables

C1 Outside Lab Data (mdl_values)

6.3.3 Upload qcanal (qaqc1) and qckey (qaqc2) data to working tables using the monitor application. From the monitor menu select:

C2 Convert QC Tables

Q2 Convert ASCII files with “conc_before_error” and “rer” fields to work tables.

Note: Duplicate object error is OKAY; hit return.

6.3.4 Verify that each result in your working table row count is the same as the corresponding ASCII files’ row count.

Note: The wanalysis table row count will be less than before if any records went to the wtic_analysis and/or wsur_analysis. The sum of all three tables should equal the number of rows in the analysis.xfer file.

6.4 Run the UPDATES Program

6.4.1 Fill in many of the blank fields in the tables by using the UNIX command:

%dmg updates

6.4.2 Perform the following steps when this program has completed:

- Type “y” (yes) for a standard report (stdrpt) print out.
- Remove MDL values from analysis results where they are not required.

- If desired enter sequence numbers to facilitate proofing of edit report using the appropriate SQL.

6.5 Groom the Data

6.5.1 Screen the data set for inconsistencies or potential problems by using the UNIX command:

%scanqry

6.5.2 Shorten the output list by using the UNIX command:

%scanlog scanquery.out.xxx>scanlog.xxx

Note: The 'out' file provides the number of problems found for that particular query with the written SQL.

6.5.3 Use the output to resolve any remaining problems with the dataset when the scanqry has finished.

6.5.4 Use the appropriate programs below or SQL commands to groom the data. Look at the current list of available checks by using the UNIX command:

%dmg info

badunits:	Checks for units of mg/L where req_analys is EPA8015 and units of µg/kgwhere matrix is SO and units not "Units" where parameter is 7,000 (pH).
blind:	Looks for potentially "blind" sample names and offers to make changes.
chgloc:	Looks for loc_id's that aren't in LOCATION table. Allows user to change loc_id's in WSAMPLE or add them to LOCATION table. - runs only on jamie - SAS.
cleanup:	Deletes unnecessary spaces in tables wsample (footnote and loc_id)and wanalysis (clp_qa_flag).
cleanwell:	Produces a printout of pertinent information regarding "hits" in sampled locations where there are not supposed to be any hits.
cntdlm:	Counts the number of delimiters on electronic files.
info:	Lists a category of commands available.
ptime:	Sets time zone field to 'PDT' or 'PST'- runs only on jamie.
qtime:	Sets time in sampled field from lab_loc_id- runs only on jamie.
rpt:	Creates a detailed edit report by log numbers or loc id.
stdrpt:	Creates an edit report of all the data in wsample and wanalysis tables.
updates:	Fills in many of the blank fields with the appropriate data in the wsample and wanalysis tables .
widow:	Runs SQL to show widowed rows in either wsample or wanalysis.
statlimitchk:	Produces a printout of pertinent information regarding "hit" in sampled locations where "hit" exceeds statistical limit.

Note: A single program can be run by command preceded with a "dmg". Use the programs independently as appropriate to make further changes to the

tables. Use interactive SQL, QBF, or the monitor application update mode if one of the above programs will not accomplish the change**.**

example: UNIX command:
%dmg badunits
[return]

6.5.5 Inform the appropriate task leader(s), WGMG Analyst, or their designee(s) if there are hits in the cleanwell program or stetlimitchk.

6.5.6 Verify new locations not in Location Table,

- Confirm location id with other team members.
- Add confirmed locations to the location table.
- Make entries in additional tables as necessary.
- Boreholes must be added to the boreholesprg table.
- Wells must be added to the well and the well-screen tables.

6.5.7 Recheck data set. Re-run the scanqry program as necessary, to check the state of the data set. The goal is for each check to result in a count of zero (0) in the SCAN log. This goal is not always possible; however all non-zero results must be understood and explained in writing on final output.

6.5.8 Run standard report. Produce standard printout to check for project codes, locations, sample dates and document control numbers on the standard report (stdrpt) program.

- Print the report.
  % mprint
  Font size 8
  Page Orientation Landscape
  Bottom Margin 2.5

6.5.9 For every treatment facility influent name that is labeled as a well name and the influent name, store in sample by the well name. Add a record to extract1well table with the same log_no, the influent name, and sampled date. There is no need to enter multiple wells going to one influent.

6.6 Account for Hard Copies for 100% Check Shipments

6.6.1 Compare hard copies with standard report.

- Sort laboratory hard copies by log number.
- Collect hard copies that are part of the current electronic shipment.
- Compare by each log number and requested analysis, if available, doing a visual scan of every page checking for unusual inclusions and exclusions.

6.6.2 Account for extra or missing hard copies. If there are any hard copies with log numbers earlier than those of the current send, check earlier shipments for missing copies and perform Step 6.6.1.

6.7 Record Data Qualifier Flags

Review validated data returned from the QC chemists to determine whether qualifier flags have been assigned.

Add electronic flags using the monitor application select:

C3 Utilities (Edit & Verify Reports)

U8 Assign (D,H,U,E, and T flags

Add all other assigned data qualifier flags to the appropriate analysis record in the analysis table, clp_qa_flag field.

Note: If an "R" flag is assigned, add an explanation in the note field of the record in the sample table.

Initial and date yellow data qualifier flag form when done.

6.8 Remove Extra Blanks

Use the cleanup program to remove extra blanks in fields: footnote and clp_qa_flag and places footnotes in alphabetical order in the tables. Using the UNIX command:

% dmg cleanup

6.9 Generate Edit Reports and Check Data

Generate edit reports including wtic_analysis and wsur_analysis and wanal_comments, if needed. Proof electronic data.

6.9.1 Select 10% or 100% of the samples for detailed data review and comparison to laboratory reports. At least one of each requested analysis type in the electronic shipment should be represented in the 10%. For new laboratories, use 100% until 3 consecutive sends have passed completely.

6.9.2 Generate an edit report of the selected samples. The selected samples can be retrieved by log_no or loc_id. From the monitor menu select:

C3 Utilities (Edit & Verify Rpts)
U2 Generate An Edit Report
E1 Sample and Analysis

and /or use the UNIX command:

% dmg rpt

6.9.3 Compare every field with the printed analytical results and verify identical content. If discrepancies between electronic and hard copy data are discovered, particularly with result and los_value, contact the analytical laboratory to confirm data.

- Request revisions with any necessary changes.
- Note requested revision in the new_data_log table.
- Make applicable changes in the work tables including a remark in the sample table note field that the revision was made on a certain date, and include your initials.

6.10 Verifications

6.10.1 Run verifications for any working table with non-zero count (wsample, wanalysis, wtic_analysis, wsur_analysis, wanal_comments) using the verification process provided by the monitor program. From monitor menu select:

C3 Utilities (Edit & Verify Rpts)
U3 Verify Work Tables (each table, respectively)
Type 'X' for "All Checks"

Note: The name(s) of output file(s). Print a screen print of this menu selection.

6.10.2 Run verifications for wqcanal and wqckey tables using the monitor application. From monitor menu select:

U3 QC Tables
U2 Verify Table Data
Type 'W' for Work Tables
Type 'X' for "All QAQC Table Checks"

Note: The name(s) of output file(s). Print a screen print of this menu selection.

6.10.3 Print the output files and include them in the final review documents.

The mprint settings should be:

Font 8
Page Orientation Landscape
Bottom Margin 2.5 inches

6.10.4 Make changes based on a careful review of the verifications. If necessary, rerun the individual verifications to show that changes have been made.

6.11 Peer Review

6.11.1 Assemble a packet of:

- Standard printout
- Edit report
- Scan log
- Verifications for all tables
- Other printouts produced by the scan (if applicable)

6.11.2 Provide packet to another DMT member for peer review for 100% proof.

6.11.3 Make necessary changes based on the reviewer's recommendations.

6.11.4 Have the reviewer make a final recheck and place their initials on data packet. Initial and date packet.

6.12 Append Data to Global Tables

Use standard monitor procedures to append wsample, wanalysis, wtic_analysis, wsur_analysis and wanal_comments tables.

6.12.1 Select from monitor menu:

C3 Utilities (Edit & Verify Rpts)
U4 Append Work to Global Tables
A1 Sample, Analysis, and Anal_Comments Tables

6.12.2 From the monitor menu select:

C3 Utilities (Edit & Verify Rpts)
U4 Append Work to Global Tables
A7 append TIC and SUR records

6.12.3 From the monitor menu select:

U3 QC Tables

U6 Append QC work table data to QC global tables

6.12.4 Print the appropriate append files, appendticanl.log and the appendqc.log files. Compare final counts with those expected (based on the known number of rows in the work tables). They should agree. If not, contact the DMT leader and/or the EPDData database administrator.

6.12.5 In the global tables, perform random retrievals to verify the records just appended are accessible.

6.13 Record the Append Activity in the Global Append Logbook

6.14 File the Append Documentation

6.14.1 File the append documentation with the printed analytical results by lab and month in the appropriate file drawer in the Division Records Center. Discard the copies of printed analytical results after one year for 100% proof analytical laboratories**,** but the append documentation should be retained as Lifetime QA Records in the Division Records Center.

7.0 QA RECORDS

7.1 All original printed analytical results reports and copies

7.2 Electronically stored records

7.3 Global Append log book

7.4 Append documentation

8.0 ATTACHMENTS

Not applicable.